Appl. No. 10/669,705
Hao Chen et al.
Reply to Office Action of July 6, 2006

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

1. (Currently amended) A method of drug discovery and development comprising:

providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;

selecting two or more molecular targets that are associated with a disease state for which the drug discovery and development are directed;

analyzing the database to identify a set of compound descriptors associated with a set of desired interactions with the two or more molecular targets;

selecting a plurality of candidate compounds as potential drugs to treat the disease state;

representing each of the candidate compounds in terms of the descriptors; and

identifying the candidate compounds with the set of compound descriptors associated with the set of desired interactions.

2. (Currently amended) The method of claim 1, wherein the plurality of candidate compounds comprise known compounds.

3. (Currently amended) The method of claim 1, wherein the analyzing step comprises reverse partitioning.

4. (Currently amended) The method of claim 1, wherein the descriptors comprise 2-D bond length descriptors.

5. (Currently amended) A method of drug discovery and development comprising:

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providing a full-rank database of interactions between a plurality of molecular targets and a plurality of compounds, wherein the database comprises a set of descriptors that describe structural features of the molecular targets and the compounds;

analyzing the database to identify a set of compound descriptors associated with both (a) a desired activity at one or more molecular targets that are associated with a disease state for which the drug discovery and development are directed and (b) an undesired activity at one or more molecular targets that are associated with undesired therapeutic effects;

representing a drug candidate in terms of the descriptors; and

determining whether the compound contains the set of compound descriptors.

6. (Currently amended) The method of claim 5, wherein the drug candidate is a known compound.

7. (Currently amended) The method of claim 5, wherein the there are multiple targets associated with the disease state.

8. (Currently amended) The method of claim 5, wherein the undesired therapeutic effect is a side effect.

9 - 37. (Canceled)

38. (New) The method of claim 5, wherein the undesired therapeutic effect is toxicity.

39. (New) The method of claim 5, wherein the undesired therapeutic effect is related to adsorption, distribution, metabolism, or elimination.

40. (New) The method of claim 5, wherein the descriptors comprise 2-D bond length descriptors.

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41. (New) The method of claim 5, wherein the analyzing step comprises reverse parititioning.